# Chemoinformatics of Ionic Liquids and Solids

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## Introduction

The **Chemical Property Viewer** (**CPV**) is an open-access portal to data of molecular and ionic compounds. The accessible data sources currently include the **ThermoML** Archive and *Axeleratio's* information snippets.
CPV implements a simple search flow: **CPV Home -> Search -> Select -> View -> Fork.**
The **View** page displays data and/or brief annotations of compound-related information. The user may "**fork"** to the associated abstracts (and full papers, typically for subscribers only) via the **D**ocument **O**bject **I**dentifier (**DOI**) or to the ThermoML source files.
CPV supports search requests with chemist-friendly input options for **chemical identifiers** including chemical compound names (synonyms, acronyms), **compound class identifiers** (names, structural notations), registry numbers, and compositional or (semi-)structural formulae. Ionic compounds can be searched by **cation-anion input**. Search methods via **ion classes** are also provided.
Here, we demonstrate and explain the abstraction of chemical names and structures using **X**ML **T**opic **M**aps (**XTM**) as the central representation of chemical identifiers. Further, the XTM representation of **associations** such as **salt/ionic-components relations** and **chemical/chemical-class relations** are discussed.

## Search Example

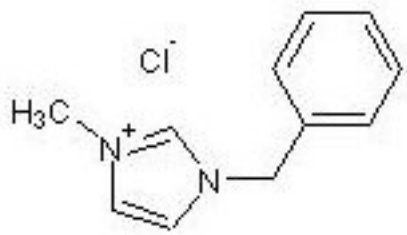
The screen shots show the search sequence for **1-benzyl-3-methylimidazolium chloride**.

**Search:**
The **cation class notation**, **1R3BzIM** (1-alkyl-3-benzylimidazolium cation), and the **anion class name**, **halogenide**, has been entered.

**Select:**
Some salts that meet the search criteria have been found. Typically such a selection set is a result of using **ionic class names/notations**, or **stoichiometric formulae** for which various isomeric compounds are possible.

**View:**
A referenced annotation regarding the **pyrolysis of 1-benzyl-3-methylimidazolium chloride** the has been located and displayed.

The example illustrates CPV's versatility in supporting users with **diverse preferences of chemical/structural nomenclature**.



# CPV Home at
# http://www.axeleratio.com/cpv

## Chemical Property Viewer

**The Chemical Property Viewer (CPV) is designed to find, browse, view and compare property data of chemical substances, mixtures, and materials. Goal of the CPV Project is to provide free, quick-by-click, and informed access to chemical information that supports advanced material science and sustainable chemistry.**

**Info & News**
:: About CPV
:: Data scope

**ThermoML**
:: Archive
:: Properties

**Ionic Liquids**
:: Getting Started
:: ILThermo
:: ThermoML Organic Salts

**Literature**
:: EnviroInfo2007 Paper

**Liability**
:: Statement
:: Disclaimer

**Contact**
:: Axel at axeleratio@yahoo.com

**Customize:** Temperature Pressure

**Select ThermoML-Archive substance by**

- Inorganic compound name
- Organic compound name
- CAS registry number
- Molecular formula

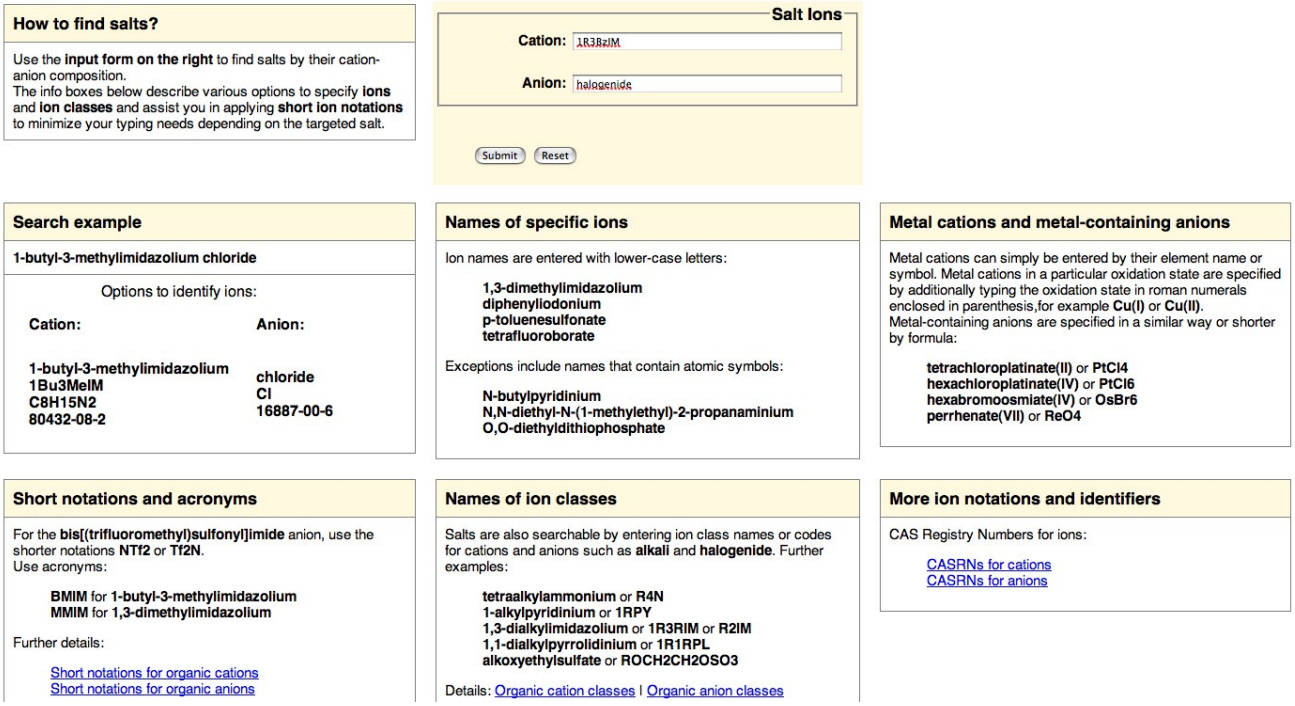
**Special substances and materials**

- Ionic liquids and solids

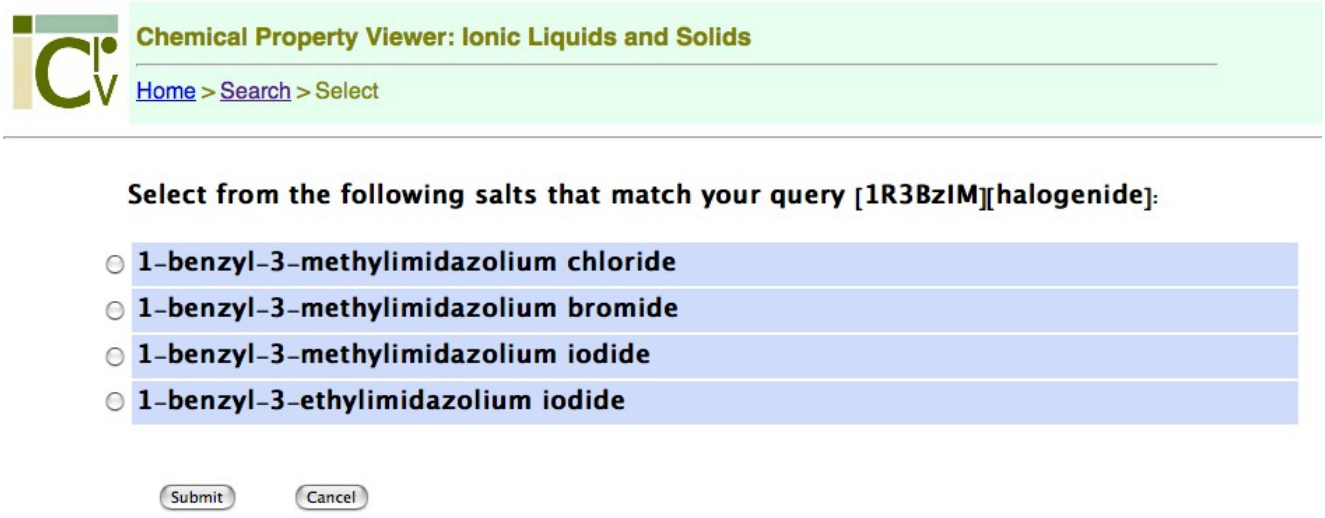
**Chemical Species**

- Cation
- Anion

# Search:




# Select:



**View:**

Chemical Property Viewer: Ionic Liquids and Solids

Home > Search > Select > View

# 1-benzyl-3-methylimidazolium chloride

$[C_{11}H_{13}N_2]^{1+}[Cl]^{1-}$ | $C_{11}H_{13}ClN_2$ => M=208.69

## Table of Search Results

Stability & Reactivity

## Stability & Reactivity

Pyrolysis: **1-benzyl-3-methylimidazolium chloride decomposes into 1-methylimidazole and 1-benzylimidazole (ratio: 1:0.67) and the corresponding organyl chlorides.** (over a period of 0.5-1.5 h at 220-260 °C with a pressure below 2 mm) [2]°


[1] Benedict K. M. Chan, Nyuk-Hon Chang and M. Ross Grimmett: The Synthesis and Thermolysis of Imidazole Quaternary Salts, *Aust. J. Chem.* 1977, *30*, 2005-2013. | DOI: 10.1071/CH9772005

[2] Table 1 on page(s) 2007 in [1]

# Behind the Scenes: XML

## Search requests in CPV are answered by directly employing data from XML files.

The CPV service uses PHP methods to load XML files, to extract and transform data, and to generate user-friendly output for display by a browser.

## Identification of ions and compounds

Chemical identification is supported by XML-encoded chemical dictionaries derived from XTM files organizing same-chemical identifiers, class memberships and, in the case of ions, associated electric charge information. Our **I**onic **I**dentification **X**TM (**IIXTM**) base currently includes over 700 ion files and 1300 salt files. Each salt files represents one ionic compound with `<variant>` nodes for chemical synonyms, registry numbers, structural notations and formulae and `<association>` nodes to relate the salt to its cation and anion components.

## Physicochemical property data from ThermoML

The **open-access ThermoML Archive**, maintained by the Thermodynamic Research Center (TRC) at the National Institute of Standards and Technology (NIST), contains XML files with experimental thermophysical and thermochemical property data for pure compounds and mixtures thereof. The data are published in peer-reviewed journals and each ThermoML file presents data of a particular journal article. Currently, property data for about 60 **ionic liquids** are available in the archive and can be viewed via CPV as a function of temperature and pressure depending on a particular property. (CPV also accesses over 1000 ThermoML-abstracted molecular compounds.)

## Chemical information from XML-encoded annotations

Whereas the current ThermoML archive is confined to five selected journals participating in the TRC/NIST effort, our XML-encoded collection of annotations is derived from a much broader spectrum of publications including journals with a defining **sustainable chemistry** (green chemistry) perspective. In addition to physicochemical data, we abstract and annotate data on safety, toxicity, electrochemistry, synthesis and potential applications including direct links (URL, **DOI**) to the reference, whenever available.

## Quantitative Structure/Property Relationships (QSPRs)

Chemical property estimation methods such as QSPRs for ionic compounds are based on properties and **ionic descriptors** of cations and anions. The IIXTM database facilitates testing and design of QSPRs and **ionic similarity** concepts. Currently, in-house software is developed for this purpose, using **SMILES notations** for ions in addition to IIXTM parameters. Further, **ionic order relations** are published online, which support design of **T**ask-**S**pecific **I**onic **L**iquids (**TSILs**) by property-driven ion selection, for example to identify critical ions for low-melting salts:
http://www.axeleratio.com/ip/QSPRs/order_ion/mpTf2N.htm .

## References

**[CPV]** Drefahl, A. "Extraction and Application of Environmentally Relevant Chemical Information from the ThermoML Archive," EnviroInfo 2007 *21st International Conference on Informatics for Environmental Protection September 12-14, 2007, Warsaw, Poland*. Pages 71 to 78 in Volume 1: Plenary and session papers. Shaker Verlag GmbH, D-52018 Aachen.
Paper: http://www.axeleratio.com/EnviroInfo2007/paper.doc
Home: http://www.axeleratio.com/cpv
Salts: http://www.axeleratio.com/cpv/salts/saltForm.php
Cations: http://www.axeleratio.com/cpv/cations/cationForm.php
Anions: http://www.axeleratio.com/cpv/anions/anionForm.php

**[ILThermo]** http://ilthermo.boulder.nist.gov/ILThermo/mainmenu.uix

**[ThermoML]** http://trc.nist.gov/ThermoML.html

**[XTM]** Park, J. (Ed.) "XML Topic Maps" Addison-Wesley, Boston, 2003.

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